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Challenges and opportunities in the Eulerian approach to numerical simulations of fixed-bed combustion of biomass

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Abstract

Fixed-bed combustion is a commonly employed technique for commercial production of heat and power from biomass and waste. In this work, the modeling challenges and opportunities within the Eulerian (averaged) approach to simulations of fixed-bed combustion systems are investigated in relation to the challenges faced within the biomass combustion area today. It is shown how the particle models for use with the Eulerian approach to numerical simulations of fixed-bed combustion should be constructed to make possible accurate predictions of the volatile release, particle heat transfer and ash slagging phenomena. A number of numerical challenges related to the accuracy and efficiency of Eulerian models for fixed-bed conversion are also identified and possible strategies to remedy them are proposed.

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Keywords: Fixed-bed combustion; Biomass conversion; Subgrid-scale modelling; Computational fluid dynamics

1. Introduction

Fixed-bed combustion is a commonly employed technique for commercial production of heat and power from biomass and waste. For biomass, fixed-bed combustion is the dominant conversion method in small-scale boilers (< 20 MW fuel input). In a typical fixed-bed furnace, the solid fuel particles are converted by the addition of air in cross-current operation, while being transported across a grate. Even though the use of this combustion technique is

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widespread, detailed knowledge about the combustion behavior is still lacking. Such detailed insight is important for a successful and efficient optimization of the fuel conversion process, with regard to parameters such as burnout, emissions, fuel flexibility and material wear. Numerical simulations are an indispensable tool in the ongoing effort to increase the possibilities to analyze fixed-bed combustion systems. Such simulations are based on one of two alternate viewpoints: either every fuel particle in the furnace is accounted for, or the behavior of the fuel particles is described only in an averaged sense. The latter viewpoint is the basis for the Eulerian modeling approach. In this approach, averaged balance equations are derived for the gas phase. For the particles, it is possible to either derive averaged balance equations as well, or to use a particle model to calculate source terms in the gas phase equations due to the (averaged) interaction with the fuel. As the information from individual particles is lost in the Eulerian approach, a number of additional modeling challenges arise that need further attention. In this work, these theoretical and numerical modeling challenges are investigated in relation to the challenges currently faced within the biomass combustion area.

Nomenclature

a	surface area per unit volume
c_p	heat capacity
eff	effective
f	face
g	gas phase
i	enumeration index
k	heat conductivity
P	cell index
S	source term
s	solid phase
T	temperature
u	velocity
V	volume
t	time
x	spatial coordinate
α	volume fraction
ρ	density
Λ	interstitial mass flux through a face

2. Types of mathematical models for fixed-bed combustion

There exist a number of different mathematical models of fixed-bed combustion of biomass. These models can be divided into two groups depending on their approach to the treatment of individual particles. In one approach, the aim is to represent every single particle present in the real system [1-4], whereas in the other approach, the ensemble of particles in the bed is treated only in average terms (represented as a solid continuum or a pseudo-fluid) [5-10]. The first approach may be referred to as a “discrete particle method” (DPM) and the latter approach is an Eulerian model. In the DPM approach, the exchange of heat and mass between the solid phase and the gas phase can be directly obtained from the individual contributions from the particles present in the computational cell. In an Eulerian approach, however, the exchange has to be modeled (for example via a submodel that performs a calculation for a representative particle [9,11,12]).

The interaction between the particles and the gas on the subgrid level (in the description of the gas phase) must however be modelled in both frameworks, since there is no computationally viable technique in which the gas flow around individual particles is fully resolved. This conclusion can for example be drawn with the aid of Fig. 1. In the left part, the total number of particles in a fixed-bed reactor is plotted as a function of the particle size and the bed volume. It is assumed that the void fraction in the bed is 63%. In the right section of Fig. 1, the total number of cells

needed to fully resolve the fields in a fixed-bed configuration is plotted as a function of the particle size for various volumes of the bed. Here, it is assumed that for the bed to be fully resolved (in terms of both the gas phase and the particle interior), 10^3 cells are needed for a volume equivalent to a cube with the size of a particle. This is a conservative estimate, given the many small voids in between particles through which the gas may pass. Finally, both graphs have a dashed red line to illustrate an approximate feasibility limit. In the left part, this line is drawn at 100,000 particles, which is a reasonable upper limit for the DPM approach. In the right part, the line illustrates 10^6 cells, which provides a hint about where a contemporary CFD multiphase simulation with simultaneous momentum, heat and mass transfer and chemical reactions would start to require computer clusters to be feasible.

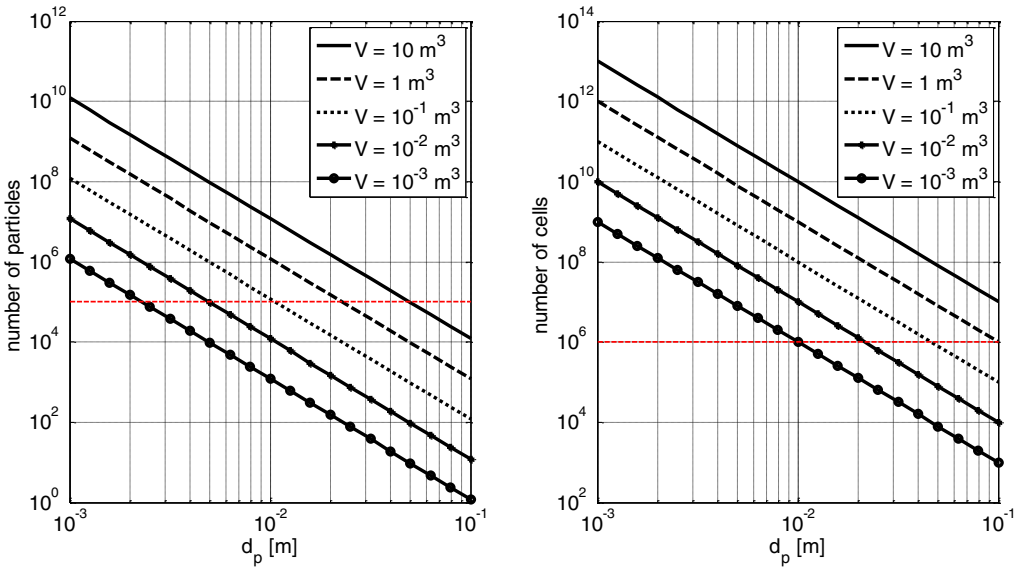

Fig. 1. Computational cost for detailed simulations of fixed-bed combustion. To the left: the total number of particles in a monodisperse system of a given size. To the right: the total number of computational cells needed for fully resolved 3D simulations. The dashed red lines illustrate the cost equivalent to 100,000 particles or 1,000,000 cells, which may be used as an approximation of the current feasibility limit.

In the Eulerian approach to fixed-bed combustion, coarse computational grids can be employed. In essence, the quality and accuracy obtainable in Eulerian simulations of fixed-bed conversion on coarse grids are limited mainly by the quality and accuracy of the subgrid models employed to describe the processes that are not explicitly resolved. Use of the Eulerian approach therefore implies a higher degree of modelling than the DPM approach, but at the gain of a lower computational cost. As illustrated in Fig. 1, the Eulerian approach is the only currently viable approach for large-scale industrial systems.

3. Theoretical challenges and opportunities in the Eulerian approach

3.1. Heat transfer due to motion of fuel particles

Heat transfer between the particles in the bed, and between the particles and the gas, is of utmost importance for the conversion processes. The drying and devolatilization of the fuel particles is largely determined by the heat transfer rate, and the ignition of the exothermic char combustion reactions also depend on the evolution of the temperature field. Heat transfer due to particle motion is of particular interest in Eulerian models, since the information about individual particles is lost in the averaging procedure. A suitable starting point for a discussion about heat transfer due to motion of fuel particles is therefore the Eulerian energy balance equation for the solid (particle) phase, which can be formulated as [5]:

$$\frac{\partial}{\partial t}\left(\alpha_s \rho_s c_{p,s} T_s\right) + M = \frac{\partial}{\partial x_i}\left(\alpha_s k_{s,eff} \frac{\partial T_s}{\partial x_i}\right) + \sum_i S_i \quad (1)$$

where the source terms in the summation on the right hand side describe the influence of the (effective) heat transfer to the particle, the heat produced (or consumed) in reactions inside the particle, and the energy transfer due to heating/cooling of gas phase products and reactants. The challenges involved in describing the effective heat conductivity in the first term on the right hand side will be discussed in Section 4.2.

The term M in equation (1) represents the energy transfer due to motion of the solid particles (i.e. during bed collapse, bed compaction or grate movement) and can be taken into account in different ways. The most general way is that of the conventional two-fluid model, to simply include a convective term (the divergence of the convective enthalpy flux due to solid phase motion), as was done by Yang et al. [13]. However, they could not find an appropriate model for the solids stress terms in their momentum balance equation for the particulate phase, and so were forced to prescribe the solid phase motion in an ad-hoc manner. Hermansson and Thunman [5] formulated their model for a moving coordinate system, so that this term vanishes. This reduction of the model complexity comes at the price of having to rescale the computational mesh to simulate the solid phase motion, and particle motion is thus modelled as discrete events. Recently, Gómez et al. [14] suggested a similar approach in which the motion of the solid phase is not solved for explicitly, but simulated in a series of discrete "compaction movements" occurring at infinite speed in between the regular Eulerian time steps. In this approach, the solid phase temperature after motion of the bed is obtained from an auxiliary iterative procedure designed to fulfill energy conservation.

In a DPM approach, the motion of the solid particles and the energy transport related to this motion can innately be taken into account, which must be considered a significant advantage. However, some of the most intricate and important mechanisms for particle motion in the fixed bed are related to aggregation and bed collapses. If these phenomena are not included in the description of the particle phase, their effect on the heat transfer and on the thermochemical conversion in the bed will also not be included. Current state-of-the-art DPM methods typically do not include such multiparticle-scale phenomena. In this respect, the Eulerian approach offers an alternative by allowing empirical models of bed collapses to be implemented without having to introduce significant changes to the description of individual particles.

3.2. Phenomena included in particle models

More than a decade ago, Thunman et al. [15] proposed a simplified discretization of biomass particles that is often used in particle models for fixed-bed combustion [4,11,12,16]. More comprehensive approaches exist [1,2,9], but require larger computational efforts. Due to the many uncertainties involved in the description of the thermochemical conversion of biomass particles, a lack of agreement between model predictions and experimental data may be caused not by a lack of detailed resolution in the model, but by phenomena not at all included. Two examples are shown in Fig. 2 by utilizing a particle model previously developed by the authors [11]. The left panel illustrates the effect of the heat of devolatilization: without taking into consideration, the comprehensive model fails to predict to the relatively slow heating of the particle interior after all the moisture has been evaporated. The right part of Fig. 2 shows the existence of an initial plateau around the boiling point of water for the particle surface temperature during almost 10 seconds, which is likely to be caused by the formation of a thin liquid film during the evaporation phase. Increased resolution of the particle interior would not recover these phenomena if not explicitly included in the particle model derivation. At the same time, when these phenomena are included in the model derivation, the correct qualitative behavior can be predicted also by simplified particle models.

The computational efficiency and robustness of the particle model is of utmost importance for numerical simulations of an entire bed to be viable [11,16,17]. Further complications may arise during drying and devolatilization due to the outflow of gases from the particles via the anisotropic wood structure. This outflow may contribute significantly to mixing and may enhance turbulence, especially at low air flows through the bed [18]. The combination of existing models for the mixing rate with a random distribution of the directions of release of volatiles and moisture [cf. 19] would provide a suitable starting point for future derivations of more advanced outflow models.

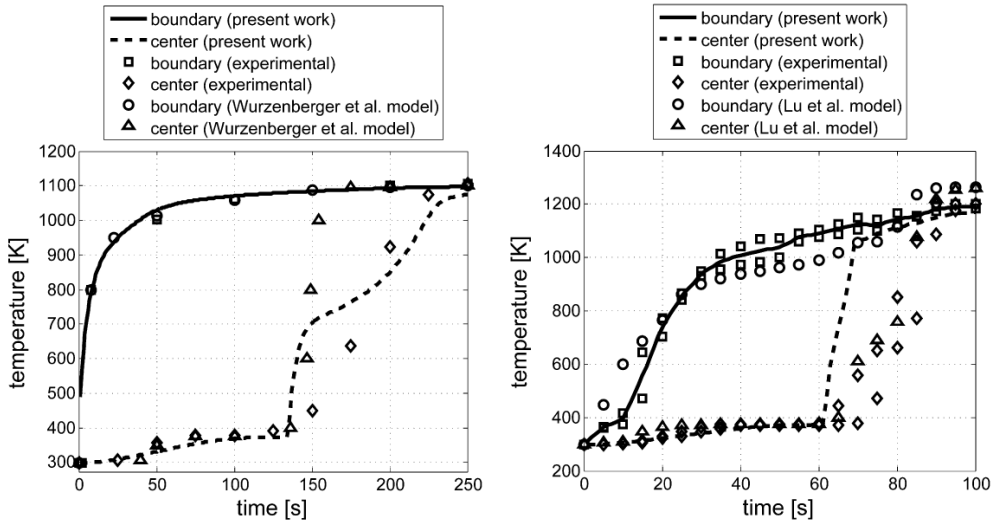

Fig. 2. Particle-scale phenomena affecting the temperature histories at the particle surface and center during the drying and devolatilization that are not captured by a finer spatial resolution of the particle interior. To the left: Slow heating of the particle interior during devolatilization for a 20 mm moist spherical wood particle at 1098 K. To the right: Probable formation of a liquid film at the surface of a 9.5 mm cylindrical (aspect ratio = 4) moist wood particle at 1276 K. Experimental data and comprehensive model predictions from Wurzenberger et al. [9] (left) and Lu et al. [20] (right). Full set of model equations for the model used in the present work are found in Ström et al. [11].

3.3. Descriptions of the interfacial area between particles and gas

A complicating factor in the derivation of particle models for fixed-bed systems is the difference between the surface area of a single particle and the surface area exposed to the gas flow for a packed bed of particles. State-of-the-art particle models are based on mass and energy balances for a single particle and typically treat the particle as one-dimensional. This approach corresponds to the assumption that gradients develop in the radial direction of a fuel particle and is realistic only if the particle is isolated, so that its entire external surface area is exposed to the gas. If two particles are packed closely together, a particle model that employs a one-dimensional description and no correction to the degree of packing will again predict radial gradients – also from the surfaces that are not exposed to the gas but to the other particle(s). This anomaly can be resolved by treating the particle as a larger body, with the same volume/mass but with a smaller surface area. An alternate way to handle this effect is to change the external transfer coefficients rather than the surface area. Such confounding of effects is likely to be one of the causes for the large uncertainties in correlations for external heat and mass transfer in fixed beds [cf. 20]. However, it is only by modeling the phenomena directly responsible for the changes to the exposed surface area (i.e. particle conversion, grate movement and bed collapses) that the dynamics of these processes can be hoped to be accurately predicted.

A novel way to handle this problem is offered by the fact that the conversion can be related to the surface area per unit volume instead of the surface area per particle [15]. Hence, current Eulerian methods could be complemented by a model for how the surface area per unit volume varies in the bed. Such a model could draw from existing techniques for interfacial area transport [21,22]. A valid starting point would be a transport equation for the local surface area per unit volume, a, of the form:

$$\frac{\partial a}{\partial t} + \frac{\partial}{\partial x_i}(a u_i) = S_a \tag{2}$$

The challenge in this approach is to correctly model the phenomena contributing to the source term (e.g. conversion and aggregation). To a first approximation, $a = 6(1-\alpha_g)/d_p$ for a packed bed of spheres [23], but in

practice a range of other factors, such as distribution of shapes and sizes, surface roughness, bed movement etc, will influence this parameter with time. An illustration of the magnitude of the changes to *a* because of these processes is shown in Fig. 3. The difference in heating rate is displayed for a piece of dry wood initially at 300K during a step change in the surface temperature to 1098K. The two cases compared are a 5x10x10 mm parallelepiped and a 10x10x10 mm parallelepiped, for which *a* differs by a factor of 4/3. Even though integral values, such as the total energy transferred, will be the same in the end, the transient behavior of the two particle systems (one large or two small particles) may be very different, especially if chemical reactions are involved. For a typical chemical reaction, a difference of tens or even hundreds of degrees corresponds to several orders of magnitude in the reaction rate. Such effects will be profound, not only on the overall rate of conversion but also on the selectivity among competing reactions.

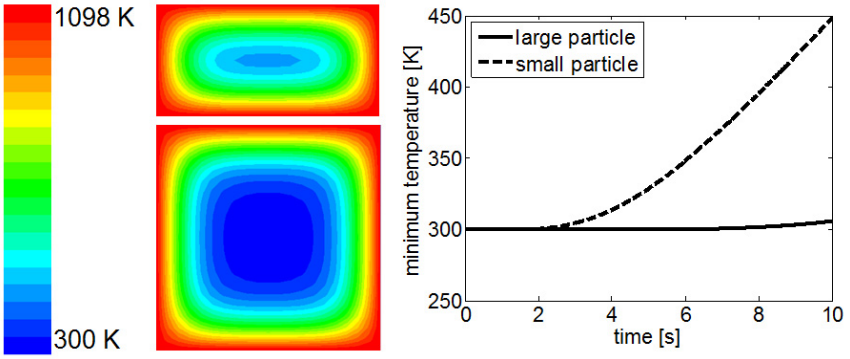

Fig. 3. Heat conduction into a solid fuel particle. To the left: temperature fields in the middle of the two particles (a 5x10x10 parallelepiped and a 10x10x10 parallelepiped) at time t = 10 s. To the right: temporal evolution of the minimum temperature inside the fuel particle (i.e. at the particle center) during the first 10 seconds. A comprehensive model is employed to solve numerically the Fourier field equation using first-order implicit time discretization ($\Delta t = 10^{-2}$ s) and a second-order central differencing scheme for the heat diffusion terms (discretized onto 20x20x20 = 8,000 grid points). The initial condition is a uniform temperature field (of 300 K) and a step change in the surface temperature to 1098K at time t = 0.

3.4. Ash slagging phenomena

With a shift towards using less traditional biofuels (e.g. agricultural crops), the fixed-bed technology will have to be adapted to accommodate effects related to the relatively low melting points of the ash in these fuels [24]. This development calls for an increased attention to the role of the ash layer in the particle model. Melting of the ash has several significant effects on the behavior of the fixed-bed combustion system. First, the molten ash facilitates particle agglomeration, which acts so as to create larger chunks of semi-converted fuel inside the bed. Bed channelling and collapses are most possibly affected by these processes. Second, the molten ash layer is less permeable to gases. The effect is especially pronounced for the diffusive transport of oxygen to the combustion front inside the particle, where the resistances to mass transport may increase by orders of magnitude [25]. Consequently, the burnout of the char takes longer time and exhibits lower peak temperatures. Furthermore, the molten ash layer has a higher thermal conductivity, which facilitates the transport of heat to and from the reaction front. Finally, constituents of the molten ash may evaporate and form precursors for particulates that may later deposit on e.g. heat exchanger surfaces or in colder section of the boiler.

The qualitative behaviour of the burnout behaviour of a single fuel particle, taking the aforementioned effects into account, is illustrated in Fig. 4. Since the phenomena pertaining to the interior of individual particles are handled by a particle submodel, the majority of these effects are as easily handled in the Eulerian framework as in a DPM approach. It is the effects of the ash on the particle agglomeration and on the macroscopic behaviour of the bed that is most challenging from a modelling perspective – modelling of these effects from “first principles” will be extremely complicated and is currently outside the scope of numerical investigations of fixed-bed conversion.

However, semi-empirical models incorporated into the Eulerian framework have already been demonstrated [5,10,14].

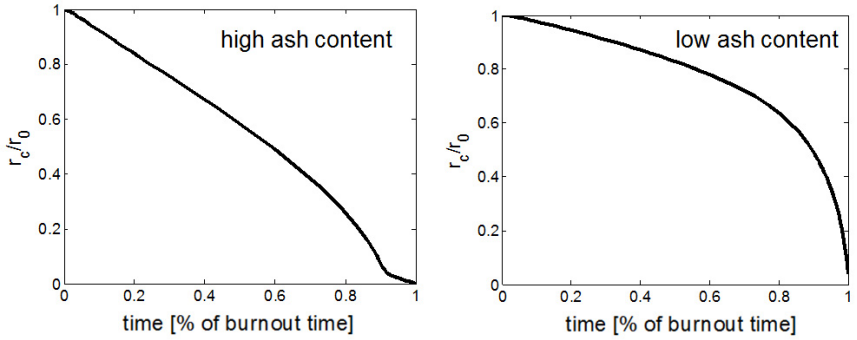

Fig. 4. Qualitative change to the fuel particle burnout behavior because of a variation in ash content. The acceleration of the conversion process resulting from the exothermic heat release for a low ash fuel (right) does not happen for a high ash fuel (left). Computations performed using the model of Chen & Kojima [25].

4. Numerical challenges and opportunities in the Eulerian approach

4.1. Mesh deformation in Eulerian simulations

Although fixed-bed furnaces are relatively simple and efficient, the use of heterogeneous fuels (such as biomass) complicates the combustion and may cause unstable operation and channeling in the fuel bed [26]. Channeling of the fuel bed is a major cause of uneven combustion, with big fluctuations and sharp spatial variations of the fuel bed temperature [7]. The process has been shown to be self-accelerating [5,7], leading to a situation where the flame front propagates much faster towards the grate than what would be predicted from an assumption of a homogeneous fuel bed.

Eulerian models for fixed-bed conversion of biomass are typically implemented into a finite-volume framework to enable computational fluid dynamics (CFD) simulations. In such implementations, particle shrinkage can be handled by a continuous rescaling of the computational mesh [5-7]. However, changing the computational mesh is associated with several numerical challenges. First, rescaling the mesh is computationally costly. When the size of a computational cell is to change, not only the nodes of the cell in question have to be moved, but all nodes of all cells above the current cell in the direction of gravity. The motion of one node must be accounted for in large parts of the geometry, making parallelization of the algorithm more complex and computationally costly. Furthermore, moving individual nodes deteriorates the quality of the mesh. In everything but trivial cases, it will introduce skewness. Highly skewed faces and cells are not acceptable and lead to inaccurate solutions or even divergence, as the equations being solved are derived based on the assumption that the cells are relatively equiangular. Deformation of the mesh in the region around the surface of the bed makes it necessary to invoke additional algorithms (introduction of new cells and/or interpolation onto a new mesh) if the bed model is to be coupled to a simulation that includes the freeboard. Such measures are both complex and computationally costly.

Another important issue is related to the fact that rescaling of the computational mesh to describe the consumption of the solid phase necessitates the introduction of additional terms to the description of the gas phase continuity equation. The commonly used version of the gas phase continuity equation is [5,10]:

$$\frac{\partial}{\partial t}\left(\alpha_g \rho_g\right) + \frac{\partial}{\partial x_i}\left(\alpha_g \rho_g u_i\right) = S_g \tag{3}$$

As the gas phase is assumed to be incompressible, this equation yields, when integrated over a cell P with volume $V(t)$ using first-order implicit time discretization:

$$\rho_g V^{n+1} \frac{{\alpha_{g,P}}^{n+1} - {\alpha_{g,P}}^{n}}{\Delta t} + \rho_g {\alpha_{g,P}}^{n+1} \frac{V^{n+1} - V^{n}}{\Delta t} + \sum_f {\alpha_{g,f}}^{n+1} \Lambda_f = S_{g,P} \quad (4)$$

When the motion of the solid phase is accounted for by scaling of the computational mesh in between Eulerian time steps, α_g must be adjusted for the procedure to conserve the mass of the gas. This adjustment of α_g produces a non-zero contribution to equation (4) via the first term. Furthermore, there will be a non-zero contribution $\rho_g \alpha_g \partial V / \partial t$ from the second term due to the mesh deformation procedure. It is straightforward to show that for a mass-conserving mesh deformation procedure, these two terms will be of equal magnitude but of opposite sign, implying that the continuity constraint is satisfied. The gas phase momentum, energy and species balance equations will have similar contributions for the same reasons. Failure to accommodate these terms results in erroneous predictions of the effects of the source terms. The numerical implications of using deforming control volumes have been largely overlooked in the literature on fixed-bed combustion, with governing equations typically given only in their differential form and with no or little supporting discussion on their discretization.

In practice, a geometrical conservation law (GCL) [27] should be invoked to guarantee the accuracy of the numerical method for moving the grid points. It has been proven that satisfying an appropriate discrete GCL is a sufficient condition for a numerical scheme to be at least first-order time-accurate on moving meshes, but also that for high-order implicit schemes to be *first-order* accurate, the corresponding *high-order* discrete GCL must be satisfied [28]. It has been shown that it is possible to derive high-order accurate temporal schemes that either respect or violate the GCL, but that to reduce the overall errors and to preserve non-linear stability the GCL should be respected [29]. An added difficulty in simulations of fixed-bed conversion is the fact that mesh deformations during a bed collapse are very large and occur on length scales equal to several grid spacings [5]. If the deformation is not resolved, but prescribed according to a bed channeling model in between two Eulerian time steps, it is also dubious to expand the description of the temporal derivative using information from several previous time levels.

Finally, diminishing cell sizes may have a bearing on the stability of the employed numerical schemes. Explicit handling of the source terms should be avoided due to the increasing cost to remain within acceptable bounds for the magnitude of the source term in relation to the (thermal) mass of the computational cell [30].

4.2. Spatial resolution in Eulerian fixed-bed simulations

The averaging technique typically used to derive Eulerian models of fixed-bed combustion is volume averaging. For a volume average of a packed bed to be physically sound, the averaging volume should be at least ten particle diameters, as shown in Fig. 5c (smaller volumes do not contain a statistically significant number of particles). On the Eulerian level of description, no additional information can later be retrieved by employing a finer grid resolution than that used in the volume averaging procedure. It is then very discomforting that it is often reported that the spatial resolution needed to obtain mesh convergent solutions is finer than the spatial scale of the particles [5,8]. In one- or two-dimensional simulations, such a fine spatial resolution may be defended by the fact that the full (unresolved) cross-section of the bed is very large in relation to the cell size used. A two-dimensional cell can then be interpreted as representing the particle properties of the entire cross-section of the bed, meaning that it will contain a statistically significant number of particle segments. In three-dimensional simulations, however, this argument does not hold. This challenge may be handled by exchanging the volume averaging for ensemble averaging [31]. Unfortunately, ensemble-averaging is in conflict with the often used approach to initialize the bed with an uneven porosity distribution [5,10]. It will therefore be necessary to develop subgrid models for the effects of porosity variations in ensemble-averaged descriptions of fixed-bed conversion to allow theoretically sound simulations using fully Eulerian methods. It should also be stressed here that the interaction of the ensemble-averaged gas with the ensemble-averaged particle is not necessarily the same as the interaction of the volume-averaged gas with the volume-averaged particle. Additional research is needed in this area of fixed-bed combustion simulations.

It is not only the Eulerian approach that is theoretically uncertain with respect to fine mesh resolution. In fact, DPM methods share similar problems. A fundamental requirement in DPM methods is that the size of a computational cell used for the description of the gas phase is significantly larger than the size of an individual particle. Otherwise, cells might be totally occupied by particles (cf. Fig. 5a), in which case exchange terms are

poorly defined and the gas phase properties of interest (velocities, temperature, species concentrations) cannot be obtained from the cell in which the particle center of mass is currently located. When properly executed, DPM methods do not require additional models for the porosity distribution, since they only deal with individual representations. Instead, DPM simulations have to be repeated with different initial conditions (e.g. initial particle packing) until statistical convergence is obtained. This convergence is however relatively straightforward for packed beds, since the gas phase cells must contain many DPM particles. A converged set of DPM simulations should ultimately produce the same result as a properly derived ensemble-averaged Eulerian method.

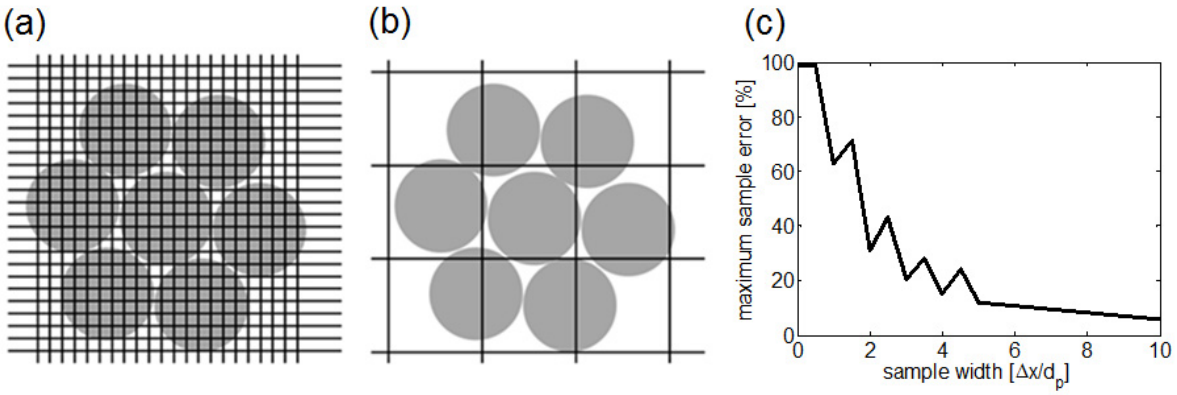

Fig. 5. Schematic illustration of different spatial resolutions in numerical simulations of fixed-bed combustion: (a) a finer resolution, where a computational cell is smaller than a typical particle; (b) a coarser resolution, where a computational cell is of the same size (or larger) as a typical particle; (c) the maximum sample error in 1,000 samples of the bed porosity as a function of the sample width (expressed in relation to the particle size).

Finally, it should also be stressed here that the effect of unresolved, local, non-linear phenomena on the overall combustion behavior remains an open issue to be addressed in fixed-bed models. As long as the flow in between particles in the bed is not fully resolved, an averaged technique is used, which results in unclosed correlations that must be modeled [32]. The cost of not addressing these issues will be the highest when dealing with detailed chemistry or when investigating the occurrence of hot spots, and is the same for Eulerian and DPM methods.

5. Summary

A number of challenges and opportunities within the Eulerian approach to numerical simulation of fixed-bed combustion of biomass have been reviewed and discussed. The main advantage of the Eulerian approach lies in its applicability to large systems (both in terms of the number of particles and the geometrical size). Since the subgrid scales are unresolved, they have to be modeled, and the Eulerian approach is therefore sensitive to the accuracy and robustness of the underlying subgrid-scale models. In general, particle models are well developed and the extensions that will become necessary in the foreseeable future (e.g. incorporations of ash slagging phenomena etc) should be possible. However, more research is needed on the descriptions of the fuel bed and the dynamics of the interface between particles and gas for heat and mass transfer, as well as on the accuracy and stability of the numerical implementations of bed channeling models. A solid theoretical foundation for future developments of three-dimensional Eulerian models will require a derivation based on ensemble-averaging rather than on volume-averaging, with an associated investigation into the applicability of existing subgrid-scale models for an ensemble-averaged description of the fixed-bed system.

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